



## Contents

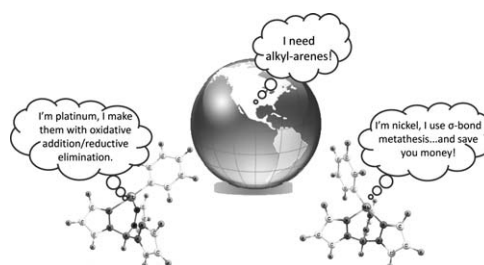
### Articles

**Thomas R. Cundari, Hector E. Gonzalez**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 1

A computational comparison of Ni<sup>II</sup> and Pt<sup>II</sup> hydrido-tris(pyrazolyl)borate supported hydroarylation catalysis

► TpNi<sup>II</sup> and TpPt<sup>II</sup> complexes had activation barriers within 2 kcal/mol of each other. TpNi<sup>II</sup> operated via a sigma-bond metathesis mechanism. ► TpPt<sup>II</sup> proceeded by an oxidative addition/reductive elimination mechanism.

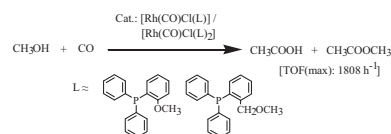


**Dipak Kumar Dutta, Biswajit Deb, Guoxiong Hua, J. Derek Woollins**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 7

Chelate and *trans* effect of P,O donor phosphine ligands on rhodium catalyzed carbonylation of methanol

► Synthesis of rhodium carbonyl complexes of P,O donor ortho-substituted triphenylphosphine ligands. Oxidative addition of CH<sub>3</sub>I to square planar Rh(I) complexes. ► Kinetic studies for the oxidative addition reactions of CH<sub>3</sub>I. Carbonylation of methanol to acetic acid and methyl acetate. ► The highest Turn Over Frequency is 1808 h<sup>-1</sup>.

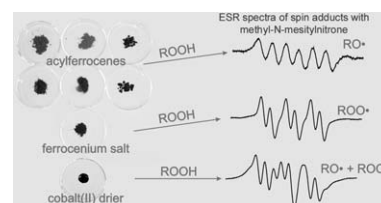


**Milan Erben, David Veselý, Jaromír Vinklárek, Jan Honzík**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 13

Acyl-substituted ferrocenes as driers for solvent-borne alkyd paints

► Acyl-substituted ferrocenes are utilizable as driers for alkyd autoxidation. ► Determination of drying time and hardness of prepared films. ► FTIR study of alkyd drying kinetics. ► Study of synergic effects in mixed drier systems. ► ESR spin trap study of t-butylhydroperoxide decomposition by ferrocenes. ► Ferrocene driers generate primarily alkoxy radicals from hydroperoxides.

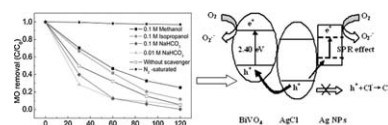


**Zhijun Zhou, Mingce Long, Weimin Cai, Jun Cai**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 22

Synthesis and photocatalytic performance of the efficient visible light photocatalyst Ag–AgCl/BiVO<sub>4</sub>

► A photocatalyst composite Ag–AgCl/BiVO<sub>4</sub> was synthesized via a photolysis–calcination method. ► Ag nanoclusters partially convert into AgCl to form the efficient Ag–AgCl photocatalyst. ► Photogenerated holes transfer to the valence band of BiVO<sub>4</sub> and O<sub>2</sub><sup>•-</sup> becomes the main active specie.

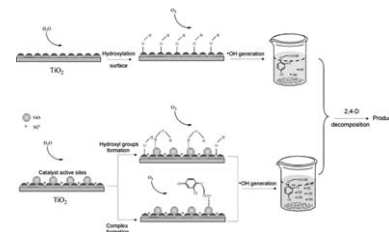


**Julia L. Rodríguez, Miguel A. Valenzuela, Francisco Pola, Hugo Tiznado, Tatiana Poznyak**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 29

Photodeposition of Ni nanoparticles on TiO<sub>2</sub> and their application in the catalytic ozonation of 2,4-dichlorophenoxyacetic acid

► Ni catalysts supported in TiO<sub>2</sub> prepared by photodeposition. ► NiO/Ni nanostructures formed after stabilization. ► Catalysts for ozonation of 2,4-dichlorophenoxyacetic acid. ► The highest catalytic ozonation rates were obtained with NiO/Ni nanostructures.

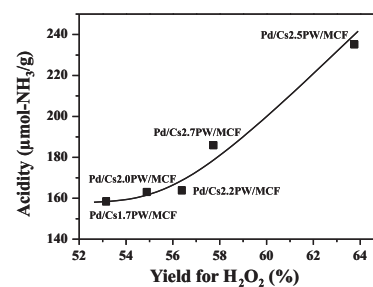


**Sunyoung Park, Jung Ho Choi, Tae Jin Kim, Young-Min Chung, Seung-Hoon Oh, In Kyu Song**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 37

Direct synthesis of hydrogen peroxide from hydrogen and oxygen over Pd/Cs<sub>x</sub>H<sub>3-x</sub>PW<sub>12</sub>O<sub>40</sub>/MCF (X = 1.7, 2.0, 2.2, 2.5, and 2.7) catalysts

► Direct synthesis of hydrogen peroxide from hydrogen and oxygen was conducted. ► Palladium catalyst supported on Cs<sub>x</sub>H<sub>3-x</sub>PW<sub>12</sub>O<sub>40</sub>/MCF was used. ► Acidity of Pd/Cs<sub>x</sub>H<sub>3-x</sub>PW<sub>12</sub>O<sub>40</sub>/MCF catalyst played an important role. ► Yield for hydrogen peroxide increased with increasing acidity of the catalyst.

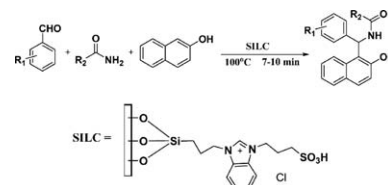


**Deepali A. Kotadia, Saurabh S. Soni**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 44

Silica gel supported –SO<sub>3</sub>H functionalised benzimidazolium based ionic liquid as a mild and effective catalyst for rapid synthesis of 1-amidoalkyl naphthols

► Supported Ionic Liquid Catalyst (SILC). ► Prepared by covalent attachment of benzimidazolium IL on surface of a solid support. ► An efficient procedure for synthesis of amidoalkyl naphthols using SILC. ► The immobilization of IL provides less leaching during the work. ► SILC provides a better catalytic site for the reaction.

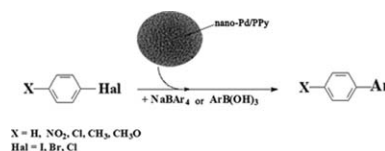


**Tatiana V. Magdesieva, Oleg M. Nikitin, Oleg A. Levitsky, Veronika A. Zinovyeva, Igor Bezverkhy, Ekaterina V. Zolotukhina, Mikhail A. Vorotyntsev**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 50

Polypyrrole–palladium nanoparticles composite as efficient catalyst for Suzuki–Miyaura coupling

- Direct redox reaction of pyrrole and Pd(NH<sub>3</sub>)<sub>4</sub>Cl<sub>2</sub> gives Pd–polypyrrole nanocomposites.
- The nanocomposites are highly efficient in Suzuki coupling. ► Morphology of the Pd/PPy hybrid material is dependent on monomer-to-oxidant ratio. Catalytic efficiency of the nanocomposite is dependent on the size of PPy globules. ► Pd nanocatalyst is active in water and can be recycled.

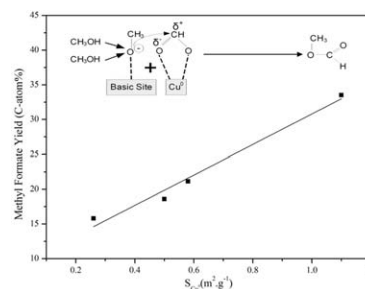


**Shahin Goodarznia, Kevin J. Smith**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 58

The effect of Cu loading on the formation of methyl formate and C<sub>2</sub>-oxygenates from CH<sub>3</sub>OH and CO over K- or Cs-promoted Cu-MgO catalysts

- The reaction of CH<sub>3</sub>OH with CO at 101 kPa over K- or Cs–Cu–MgO is reported. ► Methyl formate selectivity was >92 C-atom% at 498 and 523 K over K- or Cs–5 wt% Cu–MgO. ► At approximately constant basicity, methyl formate yield increased with Cu<sup>0</sup> surface area. ► The results suggest that methyl formate is formed on Cu<sup>0</sup> sites as opposed to Cu<sup>2+</sup> sites.

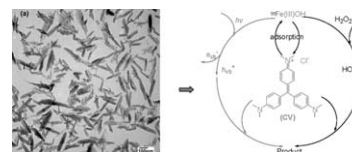


**Yulong Lin, Yu Wei, Yuhan Sun**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 67

Room-temperature synthesis and photocatalytic properties of lepidocrocite by monowavelength visible light irradiation

- Lepidocrocite was room-temperature synthesized by monowavelength LED irradiation. ► Different wavelength irradiation led to different E<sub>g</sub> value of lepidocrocite. ► γ-FeOOH obtained by blue LED irradiation has the highest Γ<sub>max</sub> and catalytic activity. ► A mechanism was suggested for the degradation of crystal violet dye.

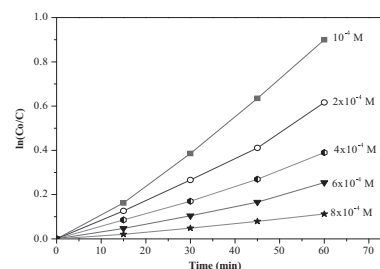


**H. Lahmar, M. Kebir, N. Nasrallah, M. Trari**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 74

Photocatalytic reduction of Cr(VI) on the new hetero-system CuCr<sub>2</sub>O<sub>4</sub>/ZnO

- The visible light activity is mediated by ZnO for the chromate reduction where 60% are reduced. ► The pseudo first order kinetic of the chromium removal obeys to the Langmuir Hinshelwood model. ► The chromate reduction is successfully achieved under direct solar radiation. ► The hetero-system CuCr<sub>2</sub>O<sub>4</sub>/ZnO favours the hydrogen formation.

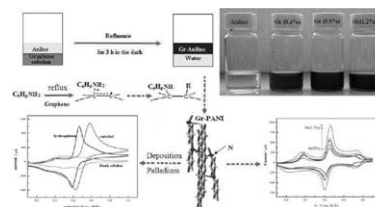


**Zhixiang Zheng, Yongling Du, Qingliang Feng, Zaihua Wang, Chunming Wang**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 80

Facile method to prepare Pd/graphene–polyaniline nanocomposite and used as new electrode material for electrochemical sensing

► The Gr colloids were prepared by the reduction of graphite oxide. ► In situ direct synthesis of graphene–aniline complex by a charge–transfer self–assembly technology. ► The Gr–aniline nanocomplex has peculiar optical property with different Gr contents. ► The graphene–polyaniline was prepared by electropolymerization of Gr–aniline. ► The Pd/Gr–PANI nanocomposite has high electro–catalytic activity for hydroquinone and catechol.

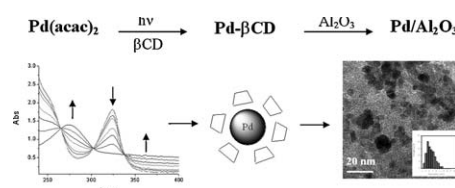


**S. Scirè, S. Giuffrida, C. Crisafulli, P.M. Riccobene, A. Pistone**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 87

Liquid phase photo-deposition in the presence of unmodified  $\beta$ -cyclodextrin: A new approach for the preparation of supported Pd catalysts

►  $\beta$ -Cyclodextrin is a reliable protecting agent to prepare Pd/ $\text{Al}_2\text{O}_3$  catalysts by LPPD. ► The role of  $\beta$ CD is to prevent the growth and aggregation of Pd particles. ► It is possible to tune the Pd particle size and the distribution by changing the  $\beta$ CD concentration. ►  $\beta$ -Cyclodextrin is easily removed from the catalyst surface by simple washing.

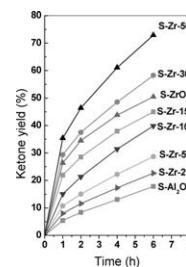


**Erming Liu, Ashley J. Locke, Ray L. Frost, Wayne N. Martens**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 95

Sulfated fibrous  $\text{ZrO}_2/\text{Al}_2\text{O}_3$  core and shell nanocomposites: A novel strong acid catalyst with hierarchically macro–mesoporous nanostructure

► We have synthesized fibrous  $\text{ZrO}_2/\text{Al}_2\text{O}_3$  nanocomposites. ► We characterised the nanocomposites by the usual materials characterisation techniques. ► The acidity of the obtained solid acids was tested by using them as catalysts for the benzoylation of toluene.

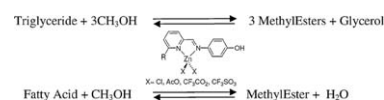


**Martino Di Serio, Giuseppina Carotenuto, Maria Elena Cucciolito, Matteo Lega, Francesco Ruffo, Riccardo Tesser, Marco Trifuoggi**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 106

Shiff base complexes of zinc(II) as catalysts for biodiesel production

► Zinc(II) complexes catalyze transesterification of soybean oil in mild conditions. ► Catalytic activity modulated by anions and substituents on bidentate ligand. ► The complexes are also active in esterification of fatty acids.

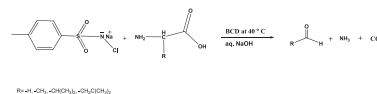


**P.A. Prasantha, N.C. Sandhya, B.K. Kempegowda, D.G. Bhadregowda, K. Mantelingu, S. Ananda, Kanchugara Koppal S. Rangappa, Manikyanahally N. Kumara**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 111

β-Cyclodextrin catalyzed oxidation of some α-amino acids with chloramine-T in alkaline medium: Kinetics and mechanistic studies

► Oxidation of α-amino acids by chloramine-T (CAT) using (β-cyclodextrin (BCD) as catalyst. ► The kinetics of reactions was fractional-order with respect to [amino acids] and [(β-cyclodextrin)]. ► The dependence of the reaction rate on temperature was studied and activation parameters were computed from Arrhenius–Eyring plots. ► The reaction mechanism and the derived rate law are consistent with the observed experimental results.

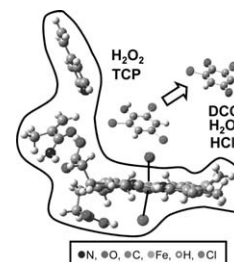


**Goretti Díaz-Díaz, M. Carmen Blanco-López, M. Jesús Lobo-Castañón, Arturo J. Miranda-Ordieres, Paulino Tuñón-Blanco**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 117

Hemo-acrylic polymers as catalyst for the oxidative dehalogenation of 2,4,6-trichlorophenol. Chloroperoxidase's mimic imprinting effects

► We synthesize hemo-acrylic polymers that mimic chloroperoxidase. ► Catalysts for the oxidative dehalogenation of 2,4,6-trichlorophenol. ► We use a combination of methacrylamide and 4-vinylpyridine as functional monomers. ► The polymer with 9:1 MA:VPY exhibited the highest catalytic efficiency. Substrate selectivity was introduced by the use of molecular imprinting technology.

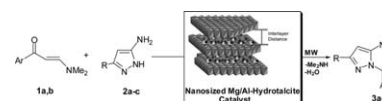


**Mohamed Mokhtar, Tamer S. Saleh, Sulaiman N. Basahel**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 122

Mg–Al hydrotalcites as efficient catalysts for aza-Michael addition reaction: A green protocol

► A hydrotalcite is presented as a potential alternative to soluble base catalysts. ► An environmentally benign method was applied to replace the classical methods. ► The microwave assisted reaction is an efficient protocol for the products in short time. ► Mg–Al hydrotalcite catalyst shows higher catalytic efficiency than its activated forms. ► A proposed mechanism for the synthesis of the aza-Michael product has been suggested for the first time.

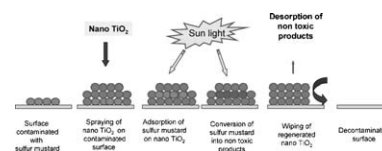


**P.V.R.K. Ramacharyulu, G.K. Prasad, K. Ganesan, Beer Singh**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 132

Photocatalytic decontamination of sulfur mustard using titania nanomaterials

► Synthesis of TiO<sub>2</sub> nanoparticles of different sizes using sol-gel method. ► Characterization of TiO<sub>2</sub> nanoparticles was done by TEM, SEM, XRD, IR, and nitrogen adsorption. ► TiO<sub>2</sub> nanoparticles exhibited better efficiency towards sulfur mustard than ZnO nanoparticles. Decontamination efficiency was found to increase with decrease in particle size. ► Percentage HD decontaminated was compared with and without irradiation.

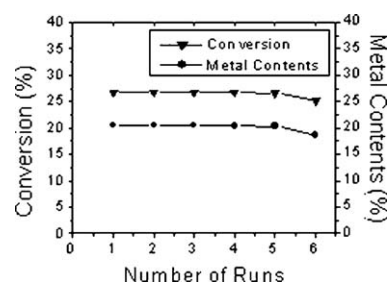


**Savita Khare, Rajendra Chokhare**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 138

Oxidation of cyclohexene catalyzed by Cu(Salen) intercalated  $\alpha$ -zirconium phosphate using dry *tert*-butylhydroperoxide

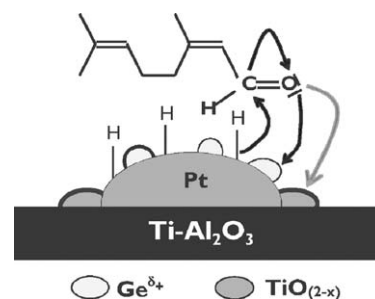
► Synthesis of a heterogeneous catalyst,  $\alpha$ -ZrP-Cu(Salen) by flexible ligand method. ► Catalyst characterized by BET, XRD, SEM, EDX, FTIR, EPR and AAS spectroscopy. ► Catalytic oxidation of cyclohexene using  $\alpha$ -ZrP-Cu(Salen)/dry TBHP system. ► Study of recycling of the catalyst up to six cycles.

**Tchirioua Ekou, Aurélien Flura, Lynda Ekou, Catherine Especel, Sébastien Royer**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 148

Selective hydrogenation of citral to unsaturated alcohols over mesoporous Pt/Ti-Al<sub>2</sub>O<sub>3</sub> catalysts. Effect of the reduction temperature and of the Ge addition

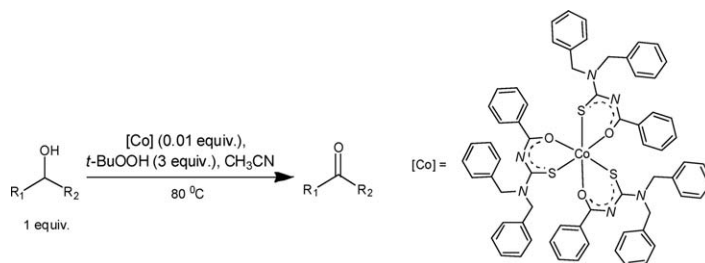
► Pt/Ti-Al<sub>2</sub>O<sub>3</sub> and Pt-Ge/Ti-Al<sub>2</sub>O<sub>3</sub> catalysts were synthesized and characterized. ► Strong metal-support interactions were evaluated using cyclohexane dehydrogenation. ► SMSI effect is more pronounced on Pt/Ti-Al<sub>2</sub>O<sub>3</sub> catalysts than on Pt/TiO<sub>2</sub> P25 sample. ► SMSI effect promotes “nerol + geraniol” selectivity during citral hydrogenation. ► Ge addition promotes “nerol + geraniol” selectivity during citral hydrogenation.

**N. Gunasekaran, P. Jerome, Seik Weng Ng, Edward R.T. Tiekink, R. Karvembu**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 156

Tris-chelate complexes of cobalt(III) with *N*-[di(alkyl/aryl)carbamothioyl] benzamide derivatives: Synthesis, crystallography and catalytic activity in TBHP oxidation of alcohols

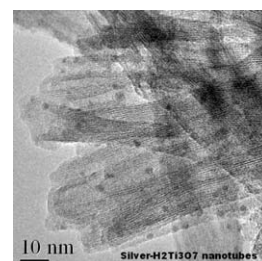
► Efficient oxidation of alcohols to carbonyl compounds in presence of *tert*-butyl hydroperoxide. Benzylic and cyclic alcohols are oxidized efficiently. ► Tris-chelate cobalt(III) complexes containing *N*-[di(alkyl/aryl)carbamothioyl]benzamide derivatives may emerge as an effective catalytic system for various organic transformations. ► Molecular structure of tris-chelate cobalt(III) complex containing *N*-[diisopropylcarbamothioyl]benzamide was determined by X-ray crystallography.

**V. Rodríguez-González, S. Obregón-Alfaro, L.M. Lozano-Sánchez, Soo-Wohn Lee**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 163

Rapid microwave-assisted synthesis of one-dimensional silver-H<sub>2</sub>Ti<sub>3</sub>O<sub>7</sub> nanotubes

► Silver-H<sub>2</sub>Ti<sub>3</sub>O<sub>7</sub> nanotubes were synthesized via microwave method in only 4 h. ► The Ag<sup>+</sup> nanoparticles promote the rapid formation of H<sub>2</sub>Ti<sub>3</sub>O<sub>7</sub> nanotubes. ► The multi-walled nanotubes have diameter of 8–10 nm and Ag<sup>+</sup> nanoparticles ~5 nm. ► The morphology-structure is related to the photocatalytic oxidation of methyl orange.

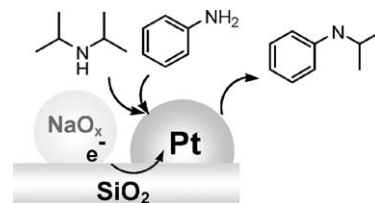


**Ken-ichi Shimizu, Katsuya Shimura, Kazuo Kato, Naoko Tamagawa, Masazumi Tamura, Atsushi Satsuma**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 171

Electronic effect of Na promotion for selective mono-*N*-alkylation of aniline with di-*iso*-propylamine by Pt/SiO<sub>2</sub> catalysts

► Moderate amount of Na-loading enhances the TOF of Pt/SiO<sub>2</sub> by a factor of 2.4. ► Na-loading increases the electron density of support oxygen atoms and consequently increases the electron density of Pt metal. ► Developed catalyst shows higher TOF than the homogeneous catalyst in the literature for the amine cross-coupling.

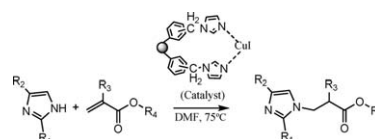


**Lixia Li, Zuliang Liu, Qilong Ling, Xiaodong Xing**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 178

Polystyrene-supported CuI-imidazole complex catalyst for aza-Michael reaction of imidazoles with  $\alpha,\beta$ -unsaturated compounds

► Polystyrene-supported CuI-imidazole complex catalyst was prepared and characterized. ► Catalysts for aza-Michael reaction of imidazoles with  $\alpha,\beta$ -unsaturated compounds. ► It showed an excellent recycling efficiency over five cycles without distinct metal leaching.

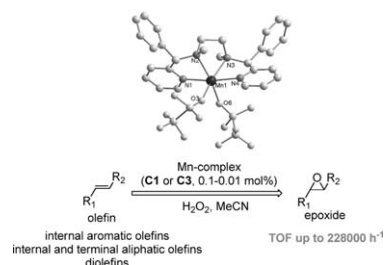


**Songjie Yu, Cheng-Xia Miao, Daqi Wang, Shoufeng Wang, Chungui Xia, Wei Sun**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 185

Mn<sup>II</sup> complexes with tetradentate N<sub>4</sub> ligands: Highly efficient catalysts for the epoxidation of olefins with H<sub>2</sub>O<sub>2</sub>

► A series of tetradentate N<sub>4</sub> Mn-complexes have been synthesized and characterized. ► The topologies of these Mn-complexes have been determined by the X-ray diffraction. ► C<sub>1</sub> and C<sub>3</sub> showed excellent selectivity, high yields and TOF with low catalyst loading for the epoxidation of a family of olefins with H<sub>2</sub>O<sub>2</sub>.

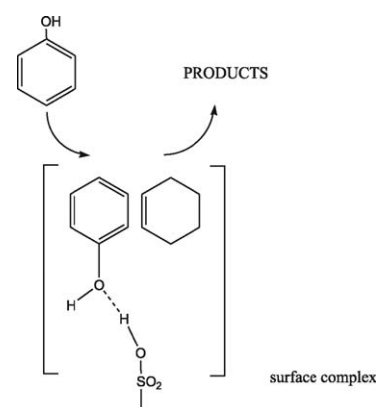


**L. Ronchin, G. Quartarone, A. Vavasori**

*Journal of Molecular Catalysis A: Chemical* 353–354 (2012) 192

Kinetics and mechanism of acid catalyzed alkylation of phenol with cyclohexene in the presence of styrene divinylbenzene sulfonic resins

► No relevant influence of the type of the sul-fonic resin on the cyclohexylation kinetics. ► Zero reaction order for cyclohexene and higher than 1 for phenol concentration. ► A consecutive adsorption equilibrium of cyclohexene on pre-adsorbed phenol occurs. ► The kinetics of cyclohexene dimerization, di-cyclohexylation, etherification and adsorption equilibria are evaluated. ► The experimental data fits a Eley-Rideal type model, which takes into account equilibria and side reactions kinetics.



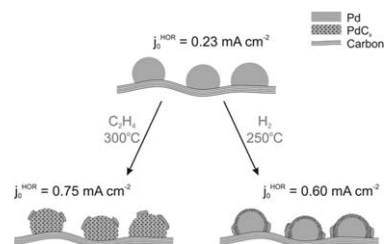


**Alexander N. Simonov, Pavel A. Pyrjaev,  
Pavel A. Simonov, Boris L. Moroz,  
Svetlana V. Cherepanova, Dmitry A. Zyuzin,  
Valery I. Bukhtiyarov, Valentin N. Parmon**

*Journal of Molecular Catalysis A: Chemical* 353–354  
(2012) 204

Enhanced catalytic activity for hydrogen electrooxidation and CO tolerance of carbon-supported non-stoichiometric palladium carbides

► Carbon-supported nanoparticles of Pd carbides as catalysts for H<sub>2</sub> electrooxidation. ► Synthesis of PdC<sub>x</sub>/C catalysts via thermal treatment of Pd/C in flowing C<sub>2</sub>H<sub>4</sub> or H<sub>2</sub>. ► Microstructure of carbon support determines plausibility of formation of Pd carbides. ► Interstitial carbon enhances catalytic activity of Pd in H<sub>2</sub> electrooxidation. ► Interstitial carbon enhances CO-tolerance of Pd during H<sub>2</sub> electrooxidation.

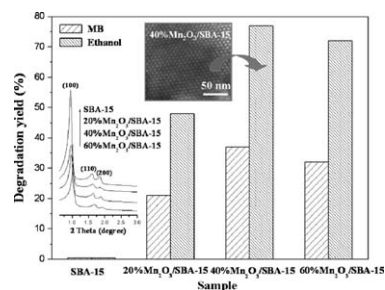


**Fenglei Cao, Hu Li, Zhenmin Xu, Jia Zhang,  
Ya Zhang, Yuning Huo**

*Journal of Molecular Catalysis A: Chemical* 353–354  
(2012) 215

Preparation of Mn<sub>2</sub>O<sub>3</sub>/SBA-15 catalyst with high loading and catalytic peroxidation for degradation of organic pollutants

► Mn<sub>2</sub>O<sub>3</sub>/SBA-15 were prepared via NH<sub>3</sub>/H<sub>2</sub>O vapor-induced internal hydrolysis process. ► Mn<sub>2</sub>O<sub>3</sub> with high loading were coated on the wall of SBA-15 without pore blockage. ► High catalytic peroxidation activity was due to well distribution of Mn<sub>2</sub>O<sub>3</sub> and large SBET. ► Acidic environment and elevated temperature could improve the catalytic activity.



**Nader Ghaffari Khaligh**

*Journal of Molecular Catalysis A: Chemical* 353–354  
(2012) 220

Erratum to "Preparation, characterization and use of 3-methyl-1-sulfonic acid imidazolium hydrogen sulfate as an eco-benign, efficient and reusable ionic liquid catalyst for the chemoselective trimethylsilyl protection of hydroxyl groups" [*J. Mol. Catal. A: Chem.* 349 (1–2) (2011) 63–70]